

2,4,6-Trimethylbenzyl cyanide

Other names:	2,4,6-Trimethylphenylacetonitrile Benzeneacetonitrile, 2,4,6-trimethyl-
Inchi:	InChI=1S/C11H13N/c1-8-6-9(2)11(4-5-12)10(3)7-8/h6-7H,4H2,1-3H3
InchiKey:	SDKQOGSGNPGPRN-UHFFFAOYSA-N
Formula:	C11H13N
SMILES:	Cc1cc(C)c(CC#N)c(C)c1
Mol. weight [g/mol]:	159.23
CAS:	34688-71-6

Physical Properties

Property code	Value	Unit	Source
gf	258.44	kJ/mol	Joback Method
hf	96.63	kJ/mol	Joback Method
hfus	18.63	kJ/mol	Joback Method
hvap	54.82	kJ/mol	Joback Method
log10ws	-3.57		Crippen Method
logp	2.678		Crippen Method
mcvol	143.470	ml/mol	McGowan Method
pc	2467.81	kPa	Joback Method
tb	594.78	K	Joback Method
tc	817.07	K	Joback Method
tf	342.70	K	Joback Method
vc	0.570	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	332.16	J/mol×K	594.78	Joback Method
cpg	344.77	J/mol×K	631.83	Joback Method
cpg	356.69	J/mol×K	668.88	Joback Method
cpg	367.93	J/mol×K	705.92	Joback Method
cpg	378.53	J/mol×K	742.97	Joback Method
cpg	388.49	J/mol×K	780.02	Joback Method
cpg	397.84	J/mol×K	817.07	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C34688716&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:

<https://www.cheméo.com/cid/79-772-8/2-4-6-Trimethylbenzyl-cyanide.pdf>

Generated by Cheméo on 2025-12-05 20:45:58.280510116 +0000 UTC m=+4715755.810550770.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.